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Marta Mendes, Ana Paula C. Ribeiro, Elisabete C.B.A. Alegria, Luísa M.D.R.S. Martins, J.L. Pombeiro

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ACCEPTED MANUSCRIPT

Liquid phase oxidation of xylenes catalyzed by the tripodal Cscorpionate iron(II) complex [FeCl₂{ κ^3 -HC(pz)₃}]

Marta Mendes,¹ Ana Paula C. Ribeiro,^{1,*} Elisabete C.B.A. Alegria,^{1,2,*} Luísa M.D.R.S. Martins,^{1,2,*} Armando J.L. Pombeiro¹

¹ Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal.

² Chemical Engineering Department, Instituto Superior de Engenharia da Lisboa, Instituto Politécnico de Lisboa, R. Conselheiro Emídio Navarro, 1959–007 Lisboa, Portugal. E-mail: *lmartins@deq.isel.ipl.pt*

Abstract

A simple and mild (room temperature) process for oxidation of *o*-, *m*- or *p*-xylene to the corresponding methylbenzyl alcohols, tolualdehydes and toluic acids, using H₂O₂ (30% aqueous solution) and the iron(II) C-scorpionate [FeCl₂{ κ^3 -HC(pz)₃}] (pz = pyrazol-1-yl) catalyst is presented. Remarkably, after 5 minutes of reaction an overall oxygenates yield of 22% (TOF = 1.3 x 10² h⁻¹) was obtained. The effects of reaction parameters, such as reaction time, temperature, amount of catalyst, type and amount of oxidant are reported and discussed.

Keywords

Xylene, oxidation, scorpionate, iron, hydrogen peroxide

Introduction

Terephthalic acid production from the oxidation of *para*-xylene is a very important process in polyester industry [1,2]. This large scale produced acid is manly used in polyethylene terephthalate (PET) manufacturing, a commodity polymer that finds use in fibers, bottles, and films. Currently, oxidation of *para*-xylene is conducted in a homogeneous catalytic system: cobalt, manganese and the highly corrosive bromide dissolved in aqueous acetic acid (Amoco process) [1]. Although very high conversions of the reactant are attained, and greener processes (*e.g.*, a spray process [3], the use of

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